Tutorial Assignment 1: Basic Statistical Mechanics

Write clearly. Answer to 4 significant figures. Marks given for units and explanation of calculations.

1. There are N identical atoms in a solid. Each particle can occupy two possible energy levels ε_1 , ε_2.

i) There are n_1 particles at energy ε_1, and n_2 at ε_2. Explain the terms macrostate and microstate in this case. [2]

ii) In terms of the number of particles n_1 at energy ε_1, and n_2 at ε_2, write down expressions for N and total energy U. [2]

iii) State the formula for Ω, the number of possible arrangements of particles in macrostate (n_1, n_2). If N = 5 and macrostate (n_1, n_2) = (3, 2), find Ω. [2]

iv) Suppose that the N and U are fixed. Using λ_1 and λ_2 respectively as multipliers, write down the Lagrangian L for maximising ln Ω. Using Stirling's approximation ($n! \approx n \ln n - n$), solve for n_1 in terms of λ_1, λ_2. [2]

v) When ln Ω is maximised, $dL = d(\ln \Omega) + \lambda_1 dN + \lambda_2 dU$ is zero for small changes in n_1, n_2 (i.e. $dL/dn_1 = 0$). Derive an expression for dU if N is fixed but U is allowed to vary. [2]

vi) From thermodynamics, $dU = TdS$ where T is temperature and S is entropy. Use (v) and the Boltzmann postulate to show that $\lambda_2 = -1/k_BT$. [2]

vii) Let A be $\exp(\lambda_1)$. From (iv) and (vi), write down the final expressions for n_1 and n_2. What is the name of this set of formulae? [2]

viii) Given that $N = N_A$, T = 1 K, ε_1 is -10^{-23} J, ε_2 is 10^{-23} J, find n_1, n_2 and U. Is the population at the higher energy level larger or smaller? [2]

ix) Suppose that we now pump 5 J of heat into the atoms. Use (ii) to find n_1, n_2. What is unusual about this result? [2]

x) Use (vii) to find the new temperature. What does (ix) suggest about negative temperatures? [2]

2. One mole of a salt at temperature T contains ions with magnetic moments. When placed in a magnetic field, the each ion has two energy levels $-\varepsilon$ and $+\varepsilon$.

i) Write down expressions for the populations of ions n_1 and n_2 respectively in these levels. Solve for n_1 and n_2 in terms of N_A, ε and T. [2]

ii) Write down an expression for total energy U in terms of ε and n_1 and n_2. Using (i), show that $U = -N_A\varepsilon \tanh(\varepsilon/k_BT)$. [2]

iii) Find the values of U when T tends to 0 and when it tends to infinity. [2]

iv) Sketch a graph of U versus T, given that the gradient is zero when $T = 0$. [2]

v) Hence sketch a graph of the heat capacity $C = dU/dT$. In most materials, C increases with T. What is unusual about this graph? [2]

vi) Use (i) to find the populations n_1 and n_2 when $T = 0$. Give the answer in terms of N_A. [2]

vii) Find the number of possible arrangements Ω when $T = 0$. Find the entropy S. [2]

viii) Use (i) to show that when T tends to infinity, an ion is equally likely to be in either level. [2]

ix) When T tends to infinity, explain why the number of possible arrangements would be 2^{N_A}. [2]

x) When T tends to infinity, show that the entropy is $N_Ak_B \ln 2$. Sketch a graph of the entropy against temperature. [2]